

2,4,6-Tricyano-1,3,5-triazine
7615-57-8 | DTXSID00274764

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.74

Global applicability domain: Outside

Local applicability domain index: 2.90e-01

Confidence level: 8.78e-01

Nearest Neighbors from the Training Set

Image not found

Amitrole

Measured: 3.09

Predicted: 3.40

Image not found

Cyanoguanidine

Measured: 3.09

Predicted: 2.93

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Diethylenetriamine

Measured: 4.47

Predicted: 4.05

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3,3'-Iminobispropanenitrile

Measured: 1.20

Predicted: 1.25

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N-(Hydroxyethyl)ethylenediamine

Measured: 2.88

Predicted: 3.29